Addendum to:
Tooele Army Depot Groundwater Flow and Contaminant Transport Model (2004)
TCE Transport Sensitivity Analysis
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Introduction

HEC and GeoTrans (2004) documented a numerical model of groundwater flow and trichloroethylene (TCE) transport at the Tooele Army Depot (TEAD). The model represents an ongoing effort to characterize and understand the dynamics of groundwater flow and TCE transport at the TEAD site. The model is generally updated annually and documentation of the changes to the model is submitted to regulatory agencies and other interested parties in April of each year. Due to time constraints for submittal to regulatory agencies, the planned TCE transport sensitivity analysis for 2004 was not completed in time for inclusion in the document. This technical memorandum documents the TCE transport sensitivity analysis and serves as an addendum to HEC and GeoTrans (2004).

Sensitivity analysis is an exercise that is conducted with a calibrated model to assess the effect of uncertainty of aquifer parameters, stresses, boundary conditions, and/or other features of the site conceptual model. During sensitivity analysis, values or representations of these factors are systematically changed within plausible ranges over the course of multiple simulations and the effect of each change noted.

Prior to conducting the TCE transport sensitivity analysis, HEC and GeoTrans (2004) performed sensitivity analysis on the groundwater flow model by varying hydraulic conductivity of specific structural features of the site, hydraulic conductivity of subsurface material of the entire site, and areal recharge. The sensitivity analysis compared the Mean Absolute Residual (MAR) for simulations where each parameter was independently varied by multiples of 0.5 and 2.0 to the calibrated model.

The sensitivity analysis for the TCE transport model involved changes to parameters that directly affect TCE movement, but do not alter the groundwater flow field. These parameters are:

- Effective porosity
- Distribution coefficient (K_d)
- Dispersivity
- Source area loading

In addition to these parameters, the model was run with two additional numerical techniques for solving the solute transport equation. Table 1 lists the parameters and factors that were varied, a qualitative description of the result, and the cumulative TCE mass removed by the groundwater extraction wells through 2003. Note that the parameters affecting the groundwater flow are not a part of this TCE transport sensitivity analysis even though they may also affect TCE transport. For example, hydraulic conductivity is not varied in this analysis even though it may affect the velocity of groundwater and in turn the migration of TCE. Groundwater flow parameters are not included in the TCE transport sensitivity analysis in order to limit the scope of the analysis.

Table 1. Summary of TCE transport model sensitivity analysis.

Parameter or factor that was varied[1]	**Parameter value(s)**	**Mass removed by extraction wells (kg)**	**Figure number**	**Qualitative description of effect**
None	Base case[2]	1003	1	
Lower effective porosity	0.75 times base	1133	2	Plume migrates farther than observed.
Higher effective porosity	1.25 times base	825	3	Plume migrates less than observed, confined to TEAD property.
Lower K_d	0.16 times base	1467	4	Plume migrates farther than observed, additional lobes present.
Higher K_d	2 times base	554	5	Plume migrates less than observed and less than high porosity simulation.
Lower Dispersivity	0.5 times base	937	6	Limited change from base case.
Higher Dispersivity	2 times base	1000	7	More dispersed plume, lower concentrations, slightly less advanced
Source area	Larger OIWL drainage system	2676	9	Concentrations significantly higher in source area and north of bedrock block. Plume migrates farther than observed.
Source area	IWL duration increase	1100	10	Limited change from base case
Solution Technique	MOC	971	11	Nearly identical to base case
Solution Technique	Finite Difference	978	12	Nearly identical to base case

[1] Note that base case parameters are used except for the parameter or factor that is varied.
[2] Base case values are: 0.20, 0.10, and 0.04 for effective porosity of most of the area, the bedrock block, and faults, respectively; 0.06 L/kg for distribution coefficient (K_d); 100 ft, 10 ft, 1ft for longitudinal, horizontal lateral, and vertical lateral dispersivity, respectively; and Total Variation Diminishing (TVD) for solution technique.

The sensitivity analysis documented in this memorandum will be used to guide the scope of the 2005 model calibration and uncertainty analysis. Recommendations for the 2005 analysis are provided in this memorandum.

Sensitivity Analysis on Parameters

The sensitivity analysis on parameters consisted of independently changing effective porosity, distribution coefficient, and dispersivity within probable ranges based on professional judgment and making model simulations with these changes. A low and high range for each parameter was evaluated using separate simulations. Thus, six sensitivity simulations were conducted on parameters. A statistical metric of goodness-of-fit (such as the MAR) was used for the groundwater flow sensitivity analysis, however, this type of metric is not used in the transport sensitivity analysis because the model was not calibrated to statistical metrics. Instead, results are compared to the 2003 modeled plume concentration (Figure 1) and to the total mass extracted.

Effective porosity affects the velocity of groundwater as it is a measure of the void space that can effectively transmit water. A change in porosity has an inverse effect on groundwater velocity that is proportional to the magnitude of the change. For example, decreasing porosity to half its original value doubles the groundwater velocity, all other parameters being unchanged. Two simulations were conducted where effective porosities were lowered to 75% of their base case values and raised to 125% of their base case values. The base case model has effective porosity values of 0.2, 0.1, and 0.04 for most of the model area, the bedrock block, and the faults, respectively. The model with the low porosities has values of 0.15, 0.075, and 0.03 for these areas. The results of this model (Figure 2) indicate that the plume has migrated farther than observed. The match immediately downgradient of the bedrock block is arguably better than the calibrated model, however the main plume extends too far and the mass extracted is higher than the base case model and calibration target. The model with the high porosities has values of 0.25 for most of the model area, 0.125 for the bedrock block, and 0.05 for the faults. The results of this model (Figure 3) indicate a less extensive plume than the base case model with the plume confined to the area of the site. The mass extracted by the treatment system is also lower than the base case result. These simulations indicate that the model is fairly sensitive to effective porosity, although the effect of changes in individual areas, such as the faults, is not clear from this analysis.

Distribution coefficient (or K_d) is a measure of the partitioning of the contaminant between liquid and solids. For fast, reversible adsorption with a linear isotherm, the retardation of the contaminant front relative to the water is described by the relation:

$$R = 1 + \rho_b/n \times K_d$$

where ρ_b is bulk mass density and n is effective porosity. A retardation factor of 1 implies that the solute will effectively move at the same velocity as the groundwater; a retardation factor of two implies that the solute will effectively move at half the velocity of groundwater. K_d is set in the base case to 0.06 L/kg, which gives a retardation factor of 1.5. Values of 0.001 L/kg and 0.12 L/kg, which give retardation factors of 1.0 and 2.0, respectively, were evaluated in the sensitivity analysis. The TCE plume for the simulation with the lower K_d is shown in Figure 4. The main plume extends farther than in the base case, with significant off-site migration. Some of the concentrations in wells north of the bedrock block are higher than the base case and therefore provide a better match to observed conditions. A middle lobe forms along Fault E while the Northeast Boundary (NEB) plume appears to deflect towards the west at the northeast end of the bedrock block and near the northeast edge of the model. The mass extracted by the model is greater than the base case, due to the increased mobility of the plume. Although there are some positive aspects of this model, the base case model appears to be more realistic. When K_d is raised (Figure 5) the plumes do not extend as far as in the base case. The match to observed data is not good, with many concentrations being underestimated. The total mass extracted in this simulation is less than for the base case, presumably due to the decreased mobility of the plume and absence of the plume in key areas. These simulations indicate that the model results are highly sensitive to K_d.

Dispersivity is a characteristic property of the medium that affects the spreading of the contaminant plume. A plume in a low dispersivity environment will generally have higher concentrations and a sharper front than a plume in a high dispersivity environment. The three components of dispersivity, longitudinal, lateral, and vertical, were set to 100 ft, 10 ft, and 1 ft, respectively, in the base case model. Two simulations were conducted with dispersivities at 50% of the base case values (50 ft, 5 ft, and 0.5 ft) and twice the base case values (200 ft, 20 ft, and 2 ft). The results of the simulation with the low dispersivities are shown in Figure 6, which are similar to the base case. The total mass extracted is slightly lower than the base case. Note that these results may contain numerical dispersion, which would mask the sharper, less dispersed plumes that would be expected from this type of change. The results of the simulation with the high dispersivity are shown in Figure 7. This simulation results in a more dispersed plume, of overall lower concentration. The mass extracted is nearly identical to the base case. The model does not appear to be sensitive to changes to dispersivity.

Sensitivity Analysis on Source Area

It was noted in HEC and GeoTrans (2004) that modeled concentrations north of the bedrock block were in many cases lower than observed. As noted during the calibration and in the sensitivity analysis on parameters, parameter adjustment was generally not effective in increasing concentrations in this particular area. Source term adjustment was identified as a possible mechanism for increasing concentrations north of the bedrock block. Two simulations were made to illustrate the sensitivity of the model to source term adjustment. The locations of the sources, as represented in the model, are shown in Figure 8. The first simulation involved increasing the area of the source that represents the drainage ditches associated with the Old Industrial Waste Lagoon (OIWL). All drainage ditches associated with the OIWL and areas where standing liquid was identified from Epic aerial photographs were assigned a similar concentration input as Ditches B and C (see Table 4 of HEC and GeoTrans, 2004). The results of this simulation, shown in Figure 9, provides a better match than the base case model in some respects—causing the plume to extend farther and increasing some of the concentrations north of the bedrock block. However, the model results show a fairly extensive area of 100 to 500 ug/L concentrations along the upgradient part of the bedrock that is an overestimate of the plume. In addition, concentrations within the bedrock block are overestimated. Total mass extracted is also overestimated for this simulation. The second simulation involved increasing the concentrations of water entering the Industrial Waste Lagoon (IWL) while using the same source areas as the base case model. Concentrations in this area were approximately doubled from the start of the IWL (1965) time period onward. The plumes resulting from this simulation (Figure 10) are not appreciably different than those of the base case. The mass extracted is slightly higher than the base case.

Sensitivity Analysis on Solution Technique

The base case simulation used the Total Variation Diminishing (TVD) technique to solve the system of equations that form the TCE transport model. This technique was selected because it strikes a balance between accuracy and simulation time. Two other solvers, the Method of Characteristics (MOC) and the Finite Difference (FD) method, were run in sensitivity simulations to determine if the choice of solution technique affects the results of the model. It was found that the results are not appreciably different (Figures 11 and 12), suggesting that any of the solvers can be used with this model.

Summary and Conclusions

Sensitivity analyses were conducted on TCE transport parameters, selected source area concentrations, and solution technique. The analyses indicate that the model is highly sensitive to changes in K_d and source concentration, moderately sensitive to changes in effective porosity, and insensitive to changes in dispersivity and the choice of solution technique. Although some of the sensitivity simulations showed some improvement over the base case in selected areas, none of the sensitivity simulations provided a better overall model than the base case. Instead, the sensitivity analysis reinforces the observation that the TEAD model is complex and that there are multiple sets of parameters that can provide acceptable matches to observed conditions. The simulations suggest that some changes in source area concentrations and inclusion of parameter zonation, if it can be physically justified, may result in a better match to observed conditions. Changes in the flow model will also change the results of the TCE transport model.

Based on the sensitivity analysis, the following recommendations are made regarding the 2005 model.

- Calibration of the groundwater flow and TCE transport models should continue to be performed in an iterative fashion. Adjustment to parameters associated with the flow model will also have an effect on the TCE transport model.
- Use of an automated parameter estimation code, such as PEST, should be attempted for calibration of the TCE transport model. This type of analysis may be faster than the current trial and error technique and allow identification of key factors that address discrete areas (such as north of the bedrock block).

- Consideration should be given to inclusion of additional parameter zonation, if it can be physically justified, to provide a better match to observed plume conditions.
- Monitoring of water levels during the Non Operation Test (NOT) Plan, where the groundwater extraction system will be shut down for a period of time, should provide useful data on the conceptual model and hydraulic conductivities. These data should be analyzed and interpreted for inclusion into the TCE transport model.
- Based on the sensitivity analysis, the location, strength, and duration of source terms are key to creating an accurate model of the TEAD. A careful review of both qualitative and quantitative data regarding the sources should be made and the results incorporated into the model.
- Predictive sensitivity analysis, or uncertainty analysis, would be useful to provide an upper and lower bound for model predictions. The scope and methods for this analysis will need to be carefully planned.

References

HEC and GeoTrans, 2004. Tooele Army Depot Groundwater Flow and Contaminant Transport Model (2004). Prepared for U.S. Army Corps of Engineers, Sacramento District. April 2004, PR-57.

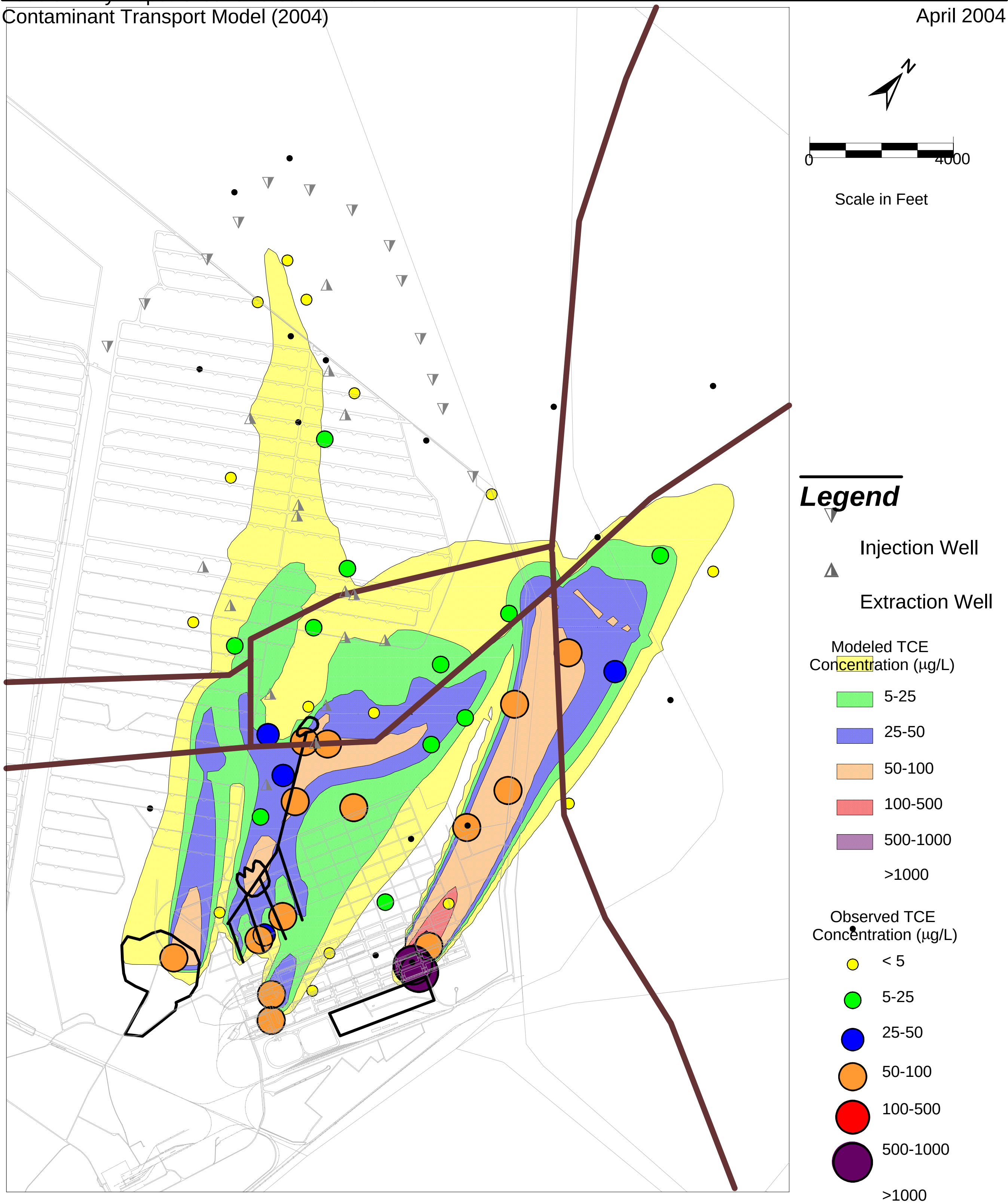

Figure 1. Modeled TCE Plume in 2003 with Observed TCE Concentrations se Case)

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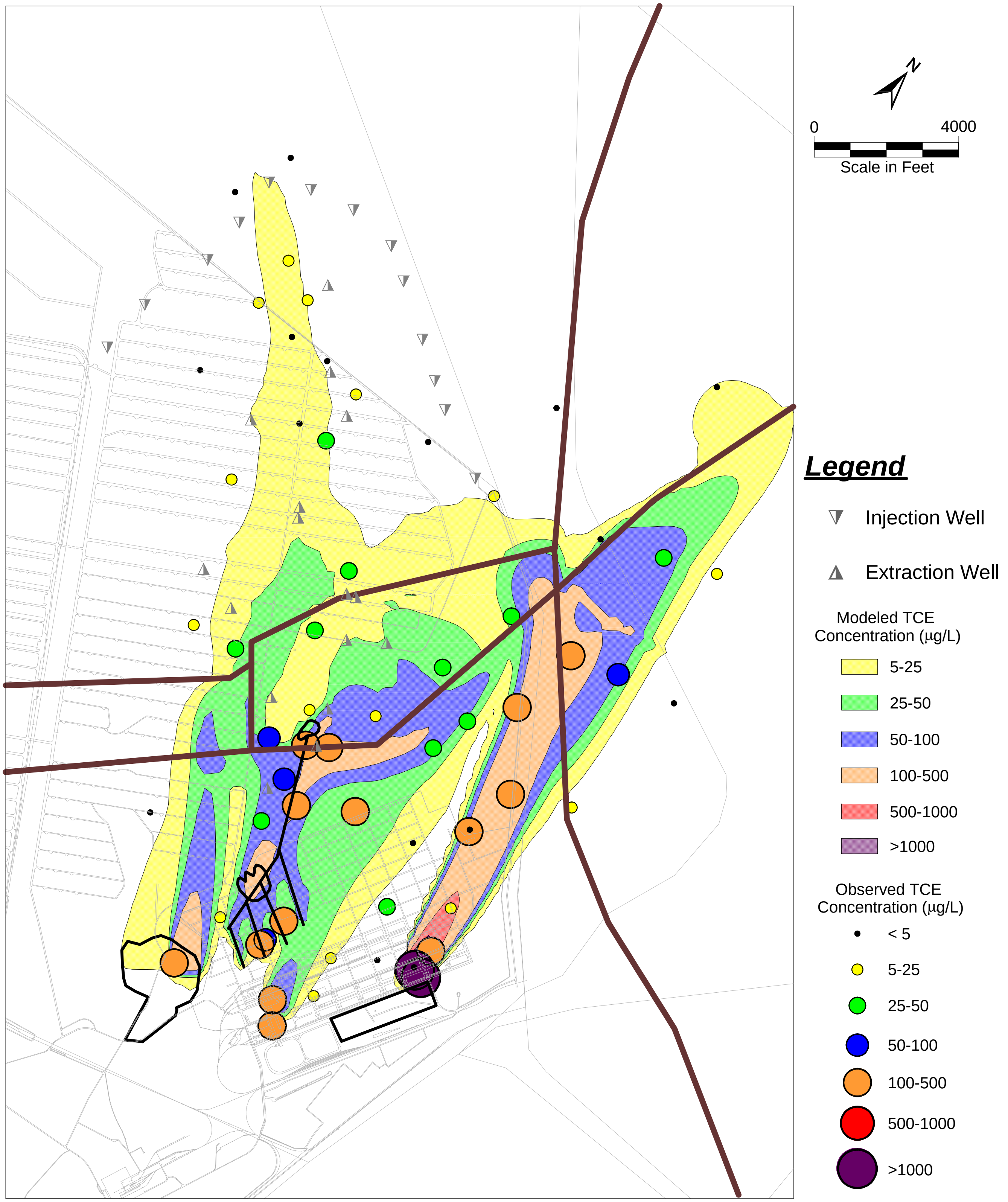

Figure 2. Modeled TCE Plume in 2003 with Observed TCE Concentrations for a Change to a Lower Porosity

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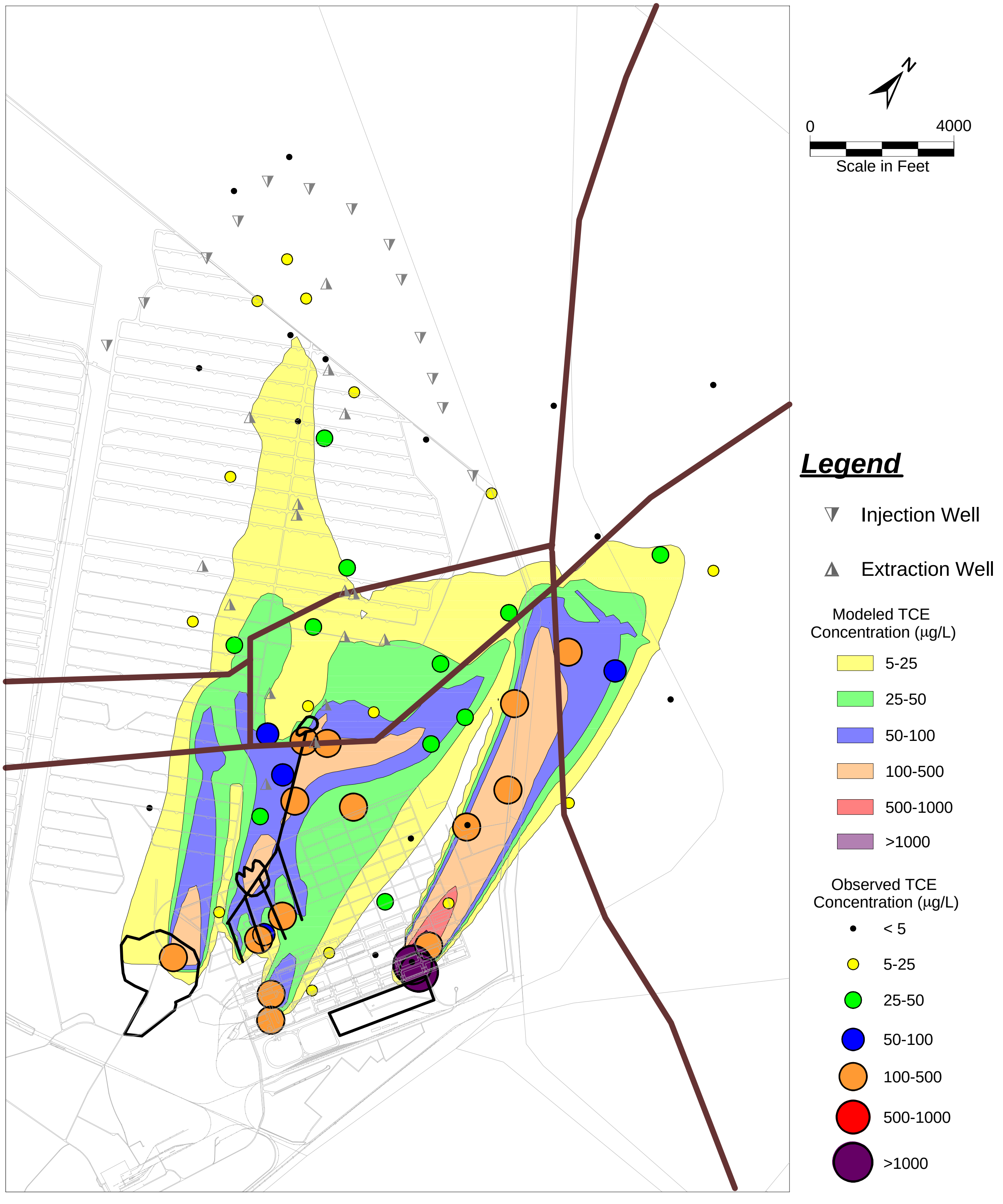

Figure 3. Modeled TCE Plume in 2003 with Observed TCE Concentrations for a Change to a Higher Porosity

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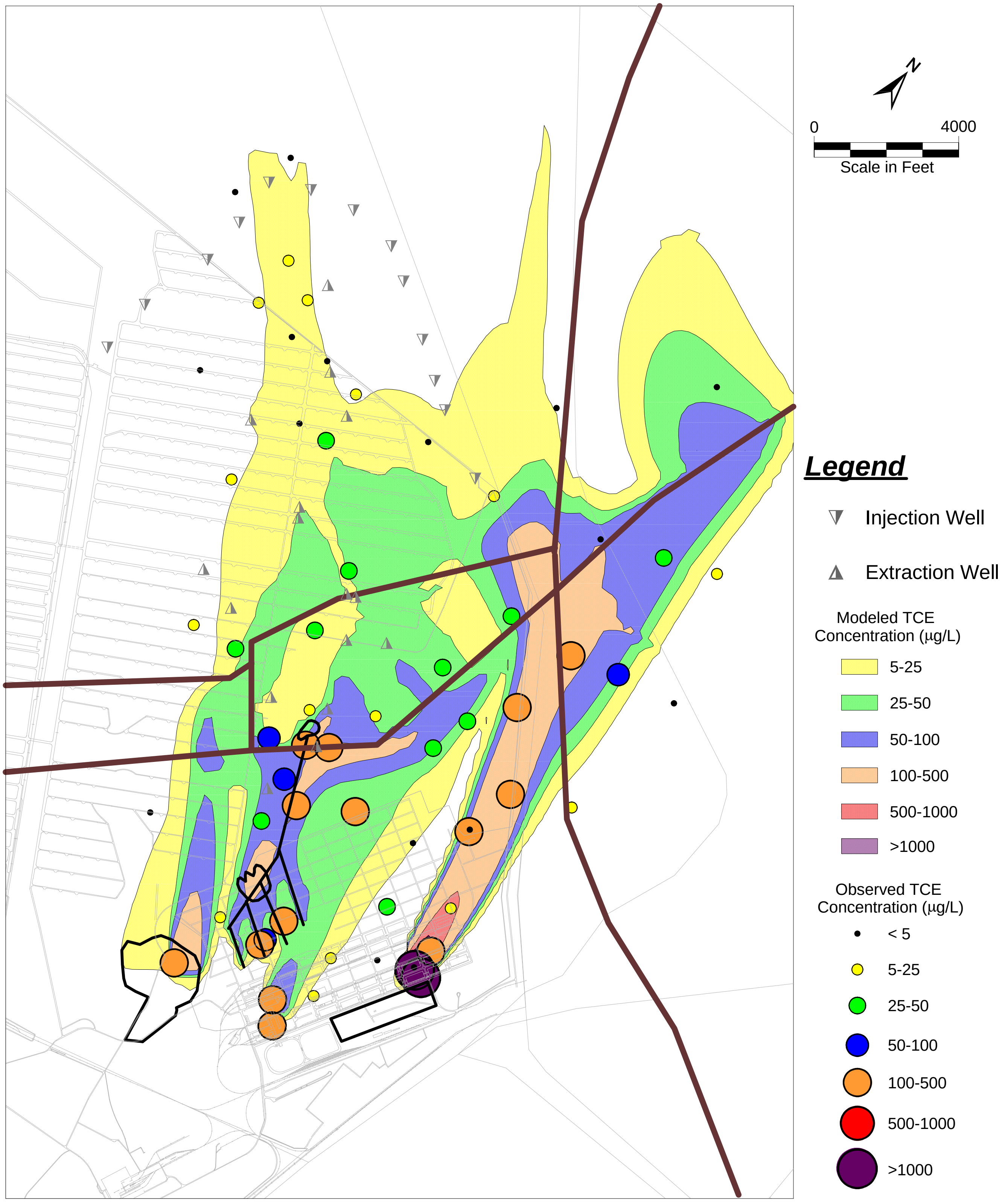

Figure 4. Modeled TCE Plume in 2003 with Observed TCE Concentrations for a Change to a Lower Kd

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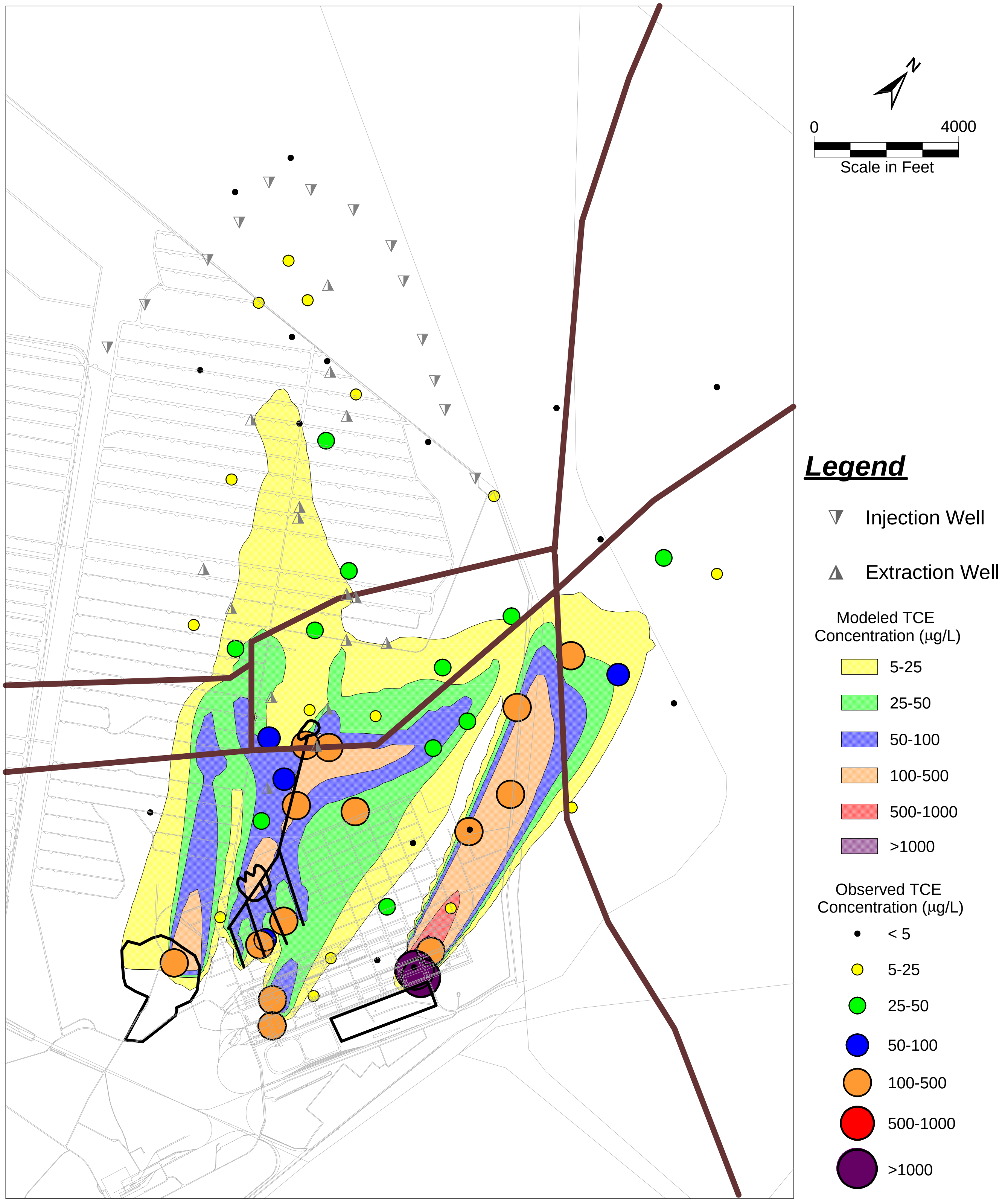

Figure 5. Modeled TCE Plume in 2003 with Observed TCE Concentrations for a Change to a Higher Kd

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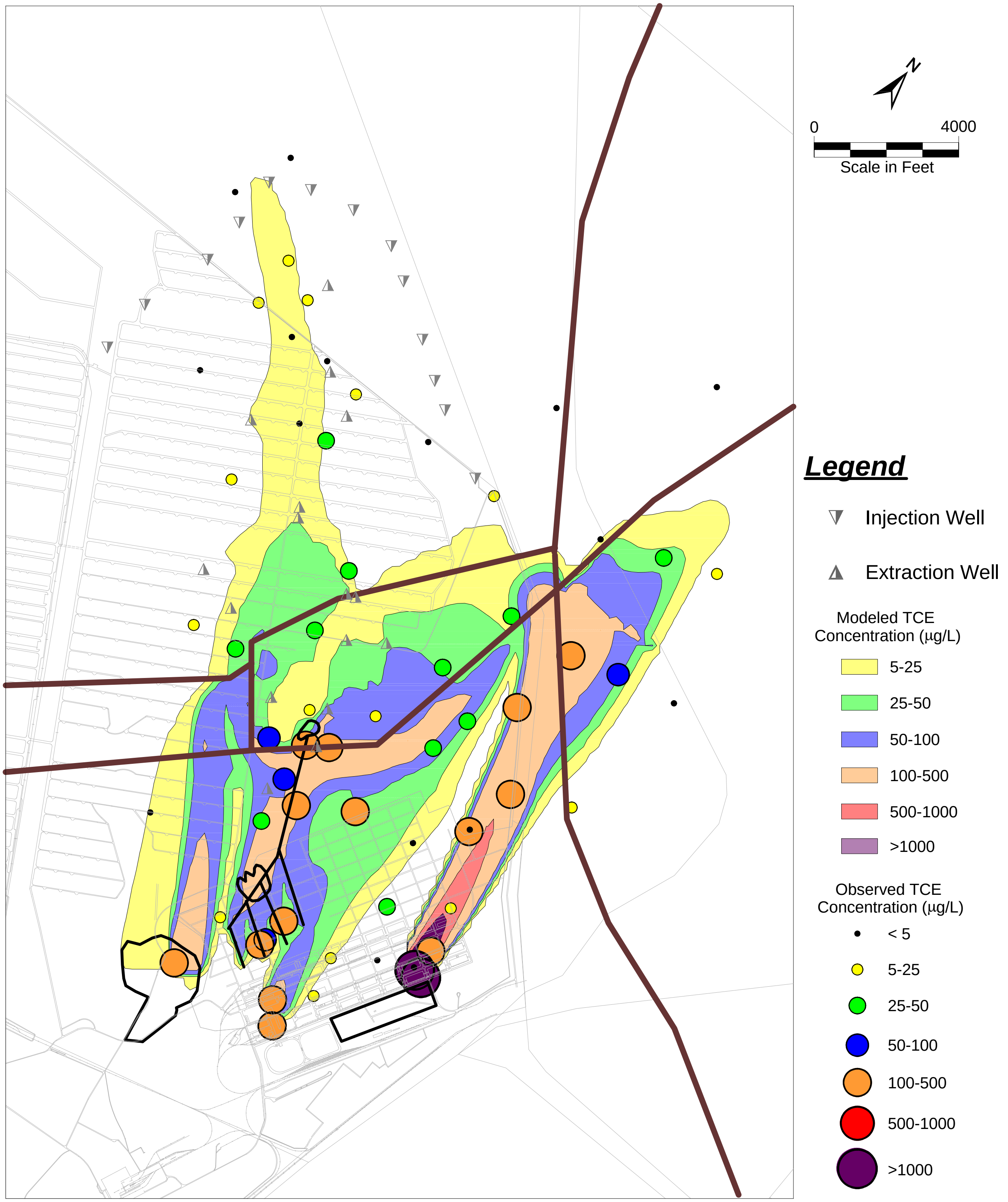

Figure 6. Modeled TCE Plume in 2003 with Observed TCE Concentrations for a Change to a Lower Dispersivity

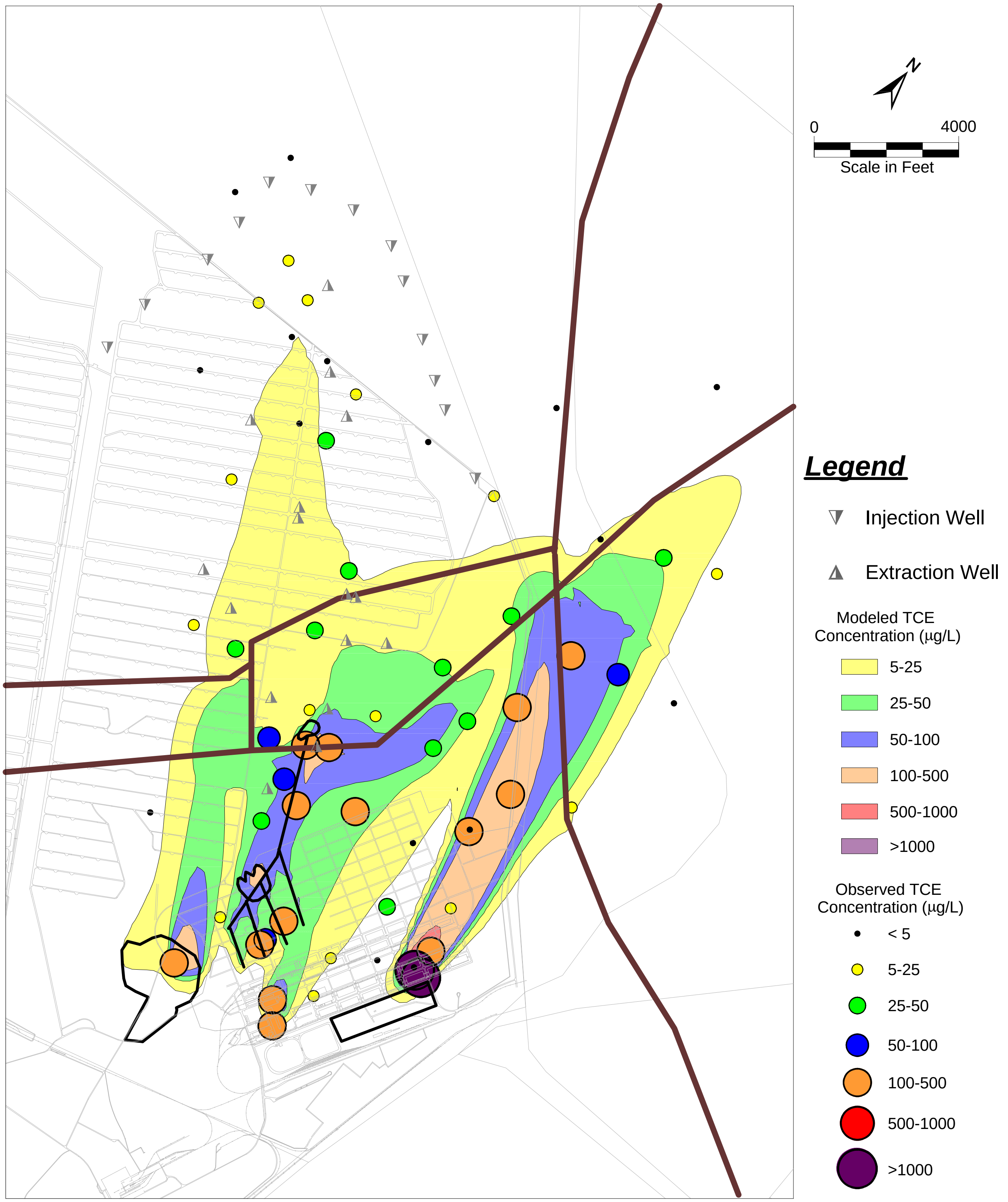

Figure 7. Modeled TCE Plume in 2003 with Observed TCE Concentrations for a Change to a Higher Dispersivity

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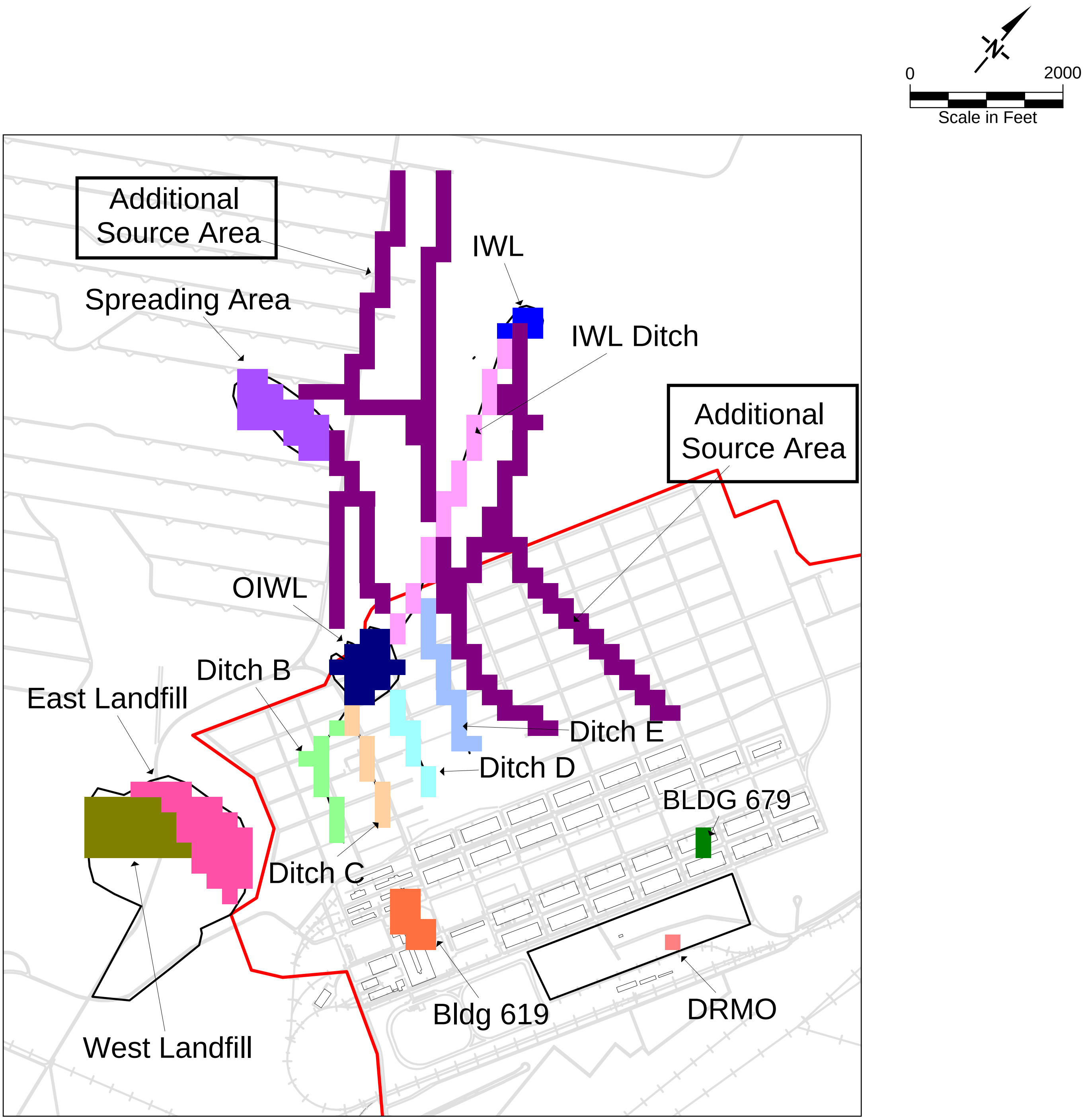

Figure 8 **TCE Source Zones, Showing Additional Source Area, (modified from HEC and GeoTrans, 2004)**

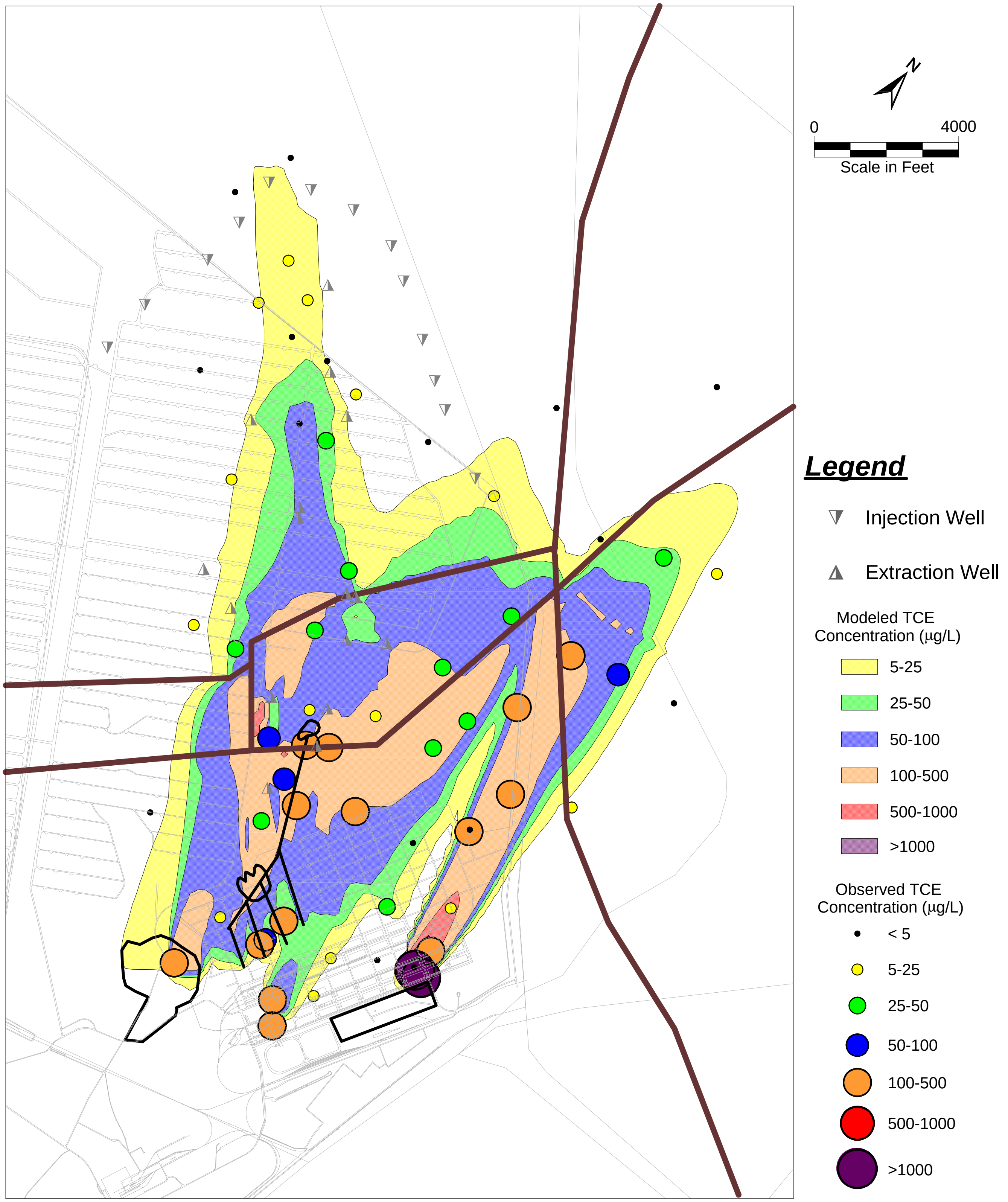

Figure 9. Modeled TCE Plume in 2003 with Observed TCE Concentrations for Inclusion of a Larger OIWL Drainage System

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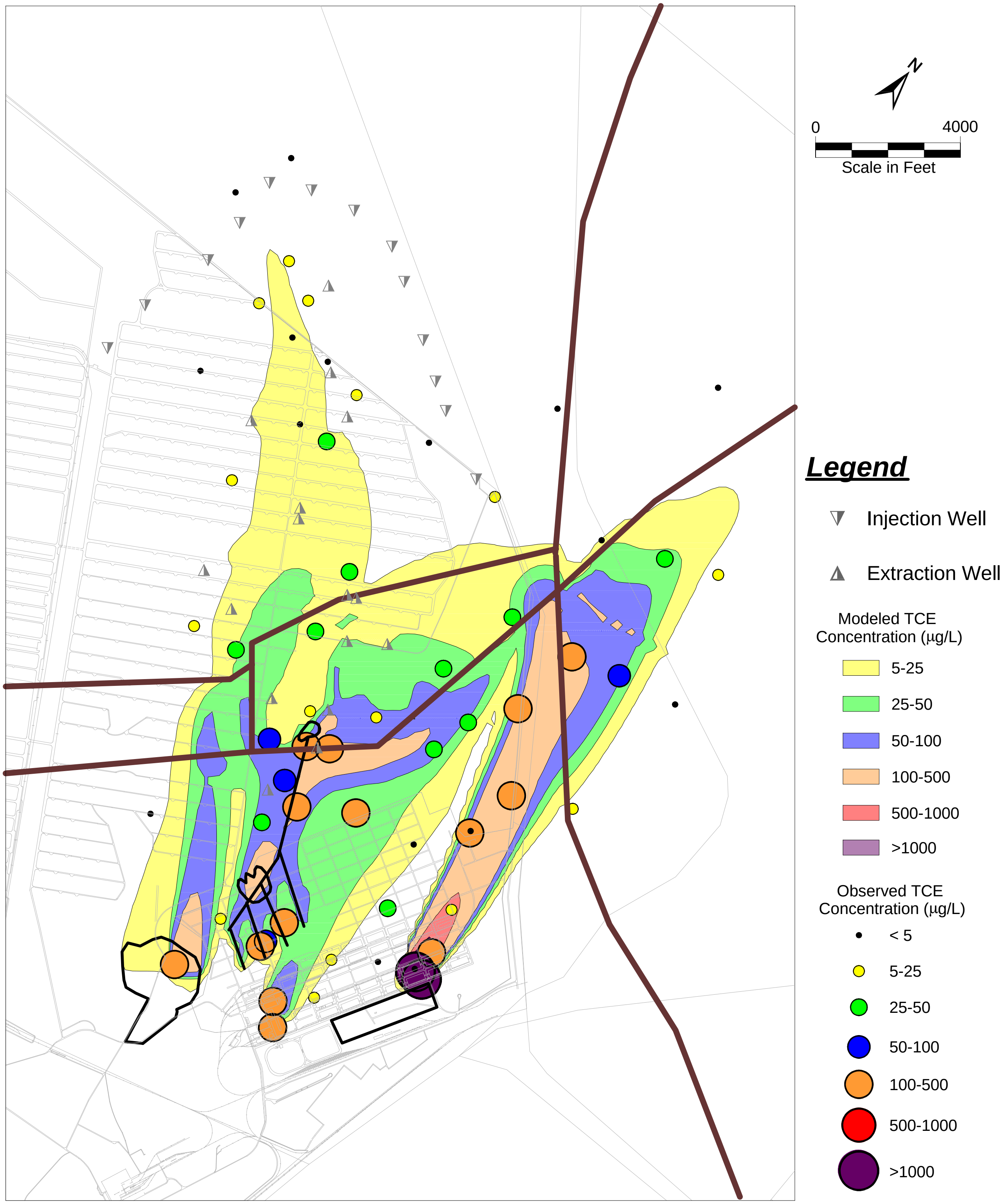

Figure 10. Modeled TCE Plume in 2003 with Observed TCE Concentrations for a Change to IWL Source Concentration

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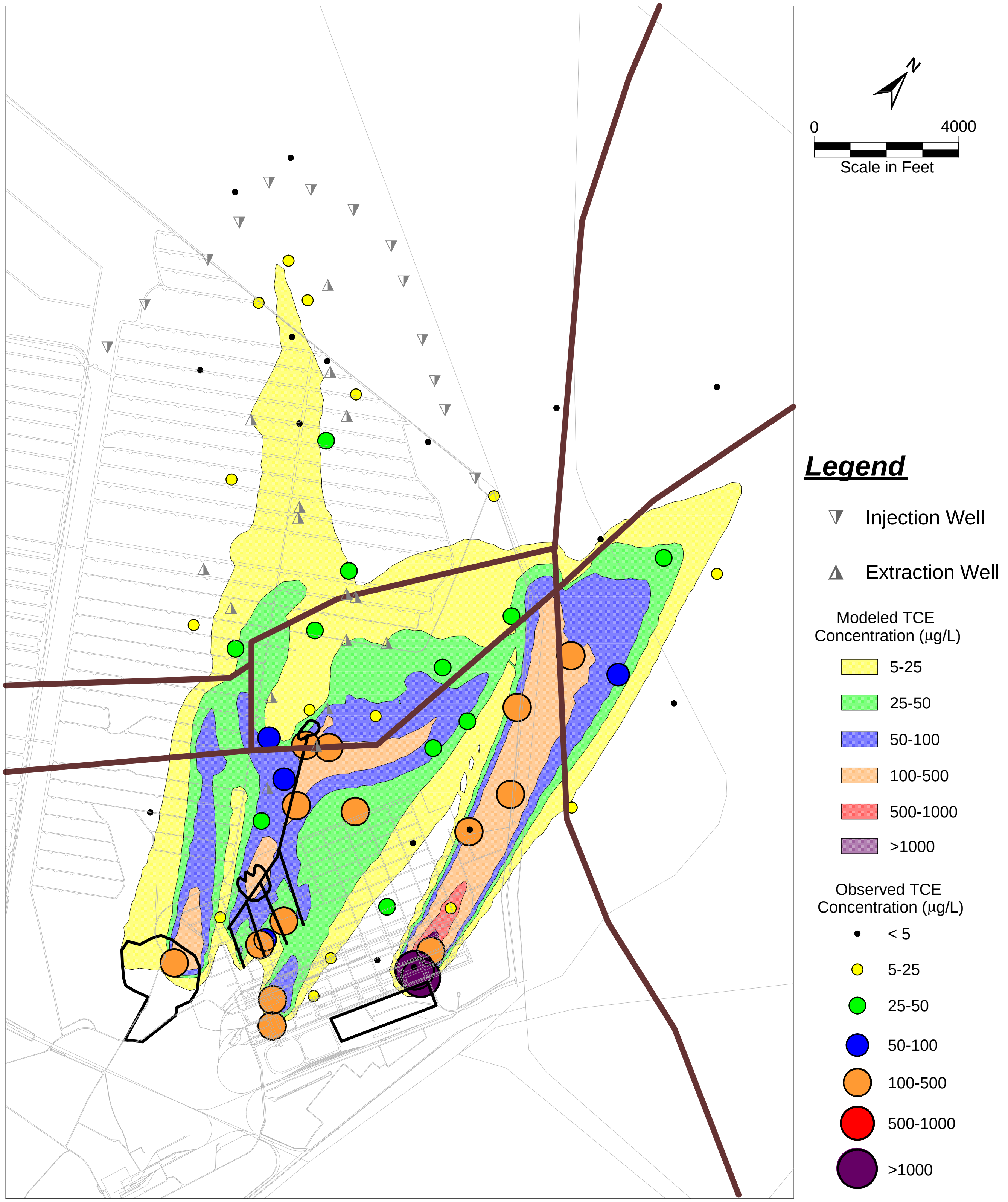

Figure 11. **Modeled TCE Plume in 2003 with Observed TCE Concentrations for a Change to the MOC Solver Technique**

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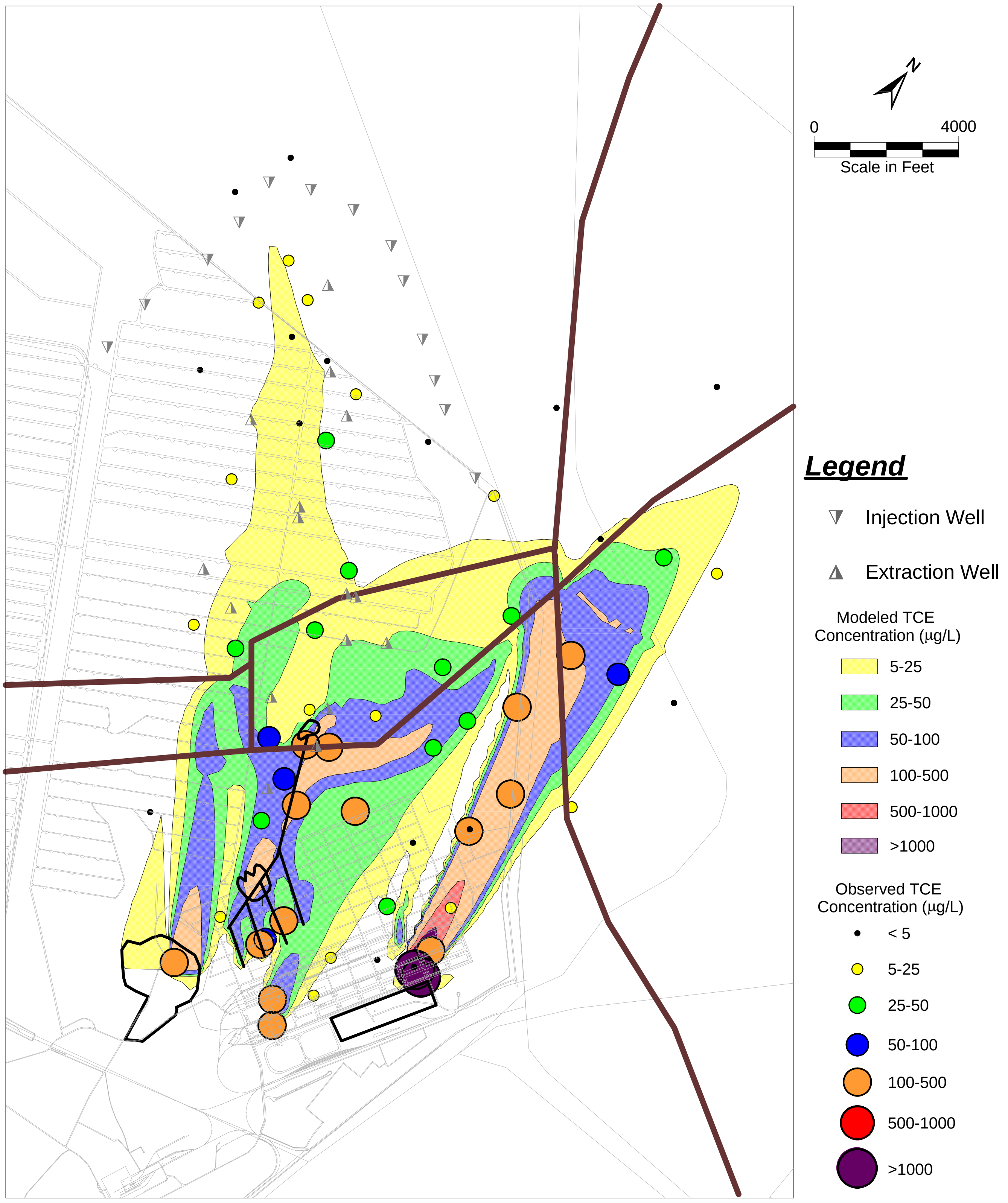

Figure 12. Modeled TCE Plume in 2003 with Observed TCE Concentrations for a Change to the Finite Difference Solution

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